



Pre-combustion Solvents and Membranes

David Luebke, NETL-RUA Research Group Leader

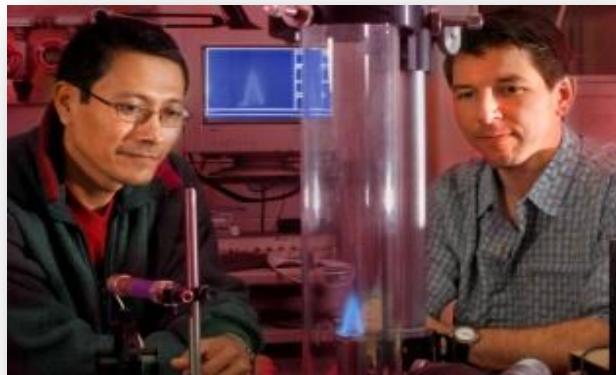
Bryan Morreale, NETL-RUA Materials Science and Engineering Focus Area Leader

August 26, 2011

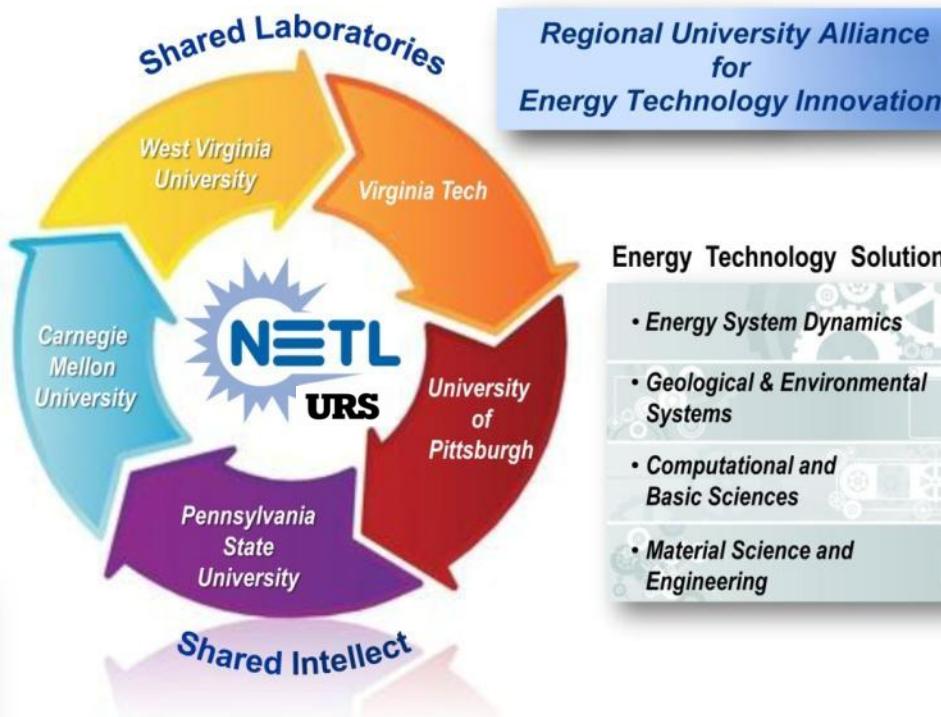


NETL's Office of Research & Development

- Use-Inspired R&D to Enable Sustainable Utilization of our Domestic Energy Resources
- Collaboration to Speed Energy Technology Discovery, Development & Deployment
- Education of the Energy Leaders for Tomorrow



Regional University Alliance



Energy Technology Solutions

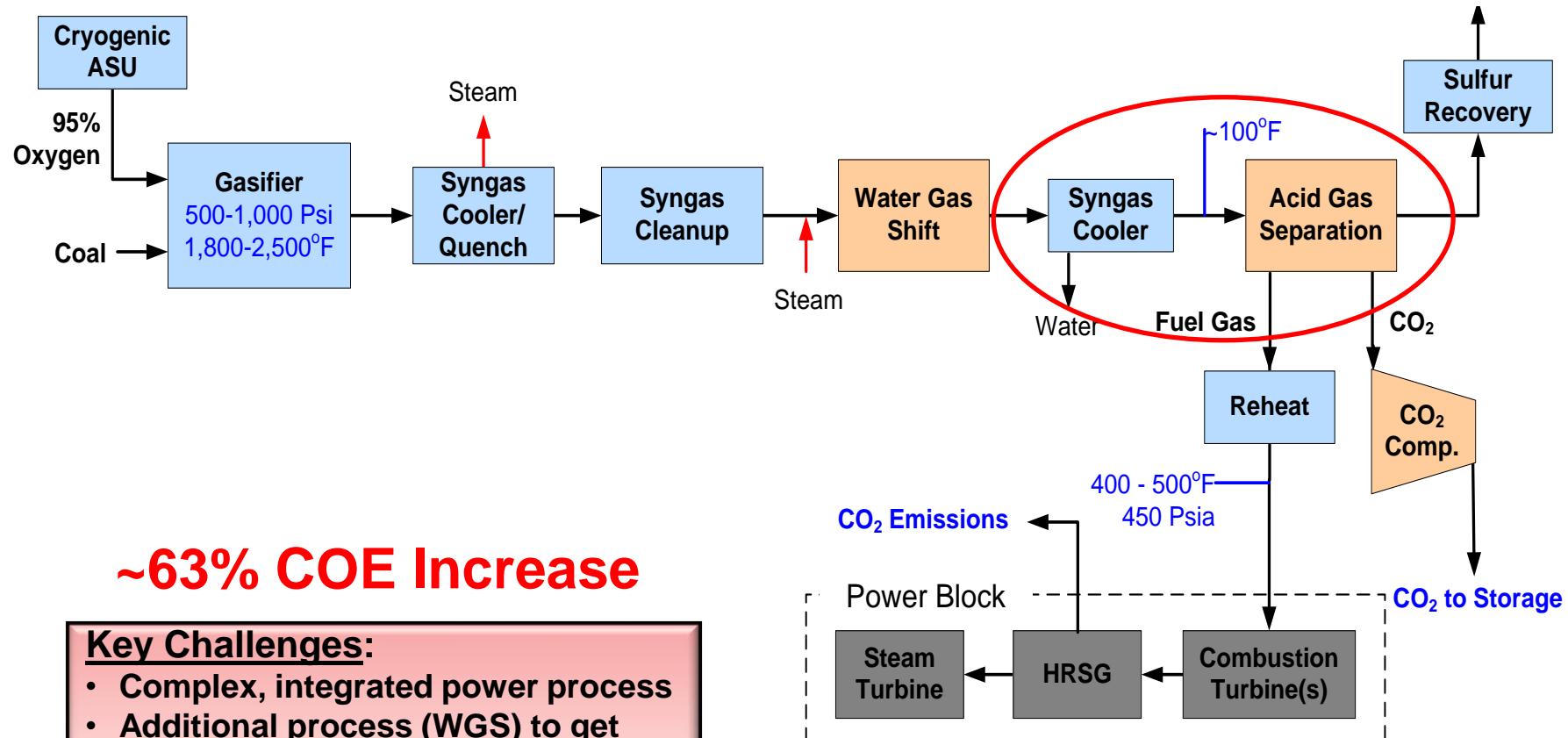
- Energy System Dynamics
- Geological & Environmental Systems
- Computational and Basic Sciences
- Material Science and Engineering



**Leveraging National Lab and University-Based Scientific and Engineering Assets
to Address Significant National Energy Issues**

IGCC Power Plant System

Pre-combustion CO₂ Scrubbing



~63% COE Increase

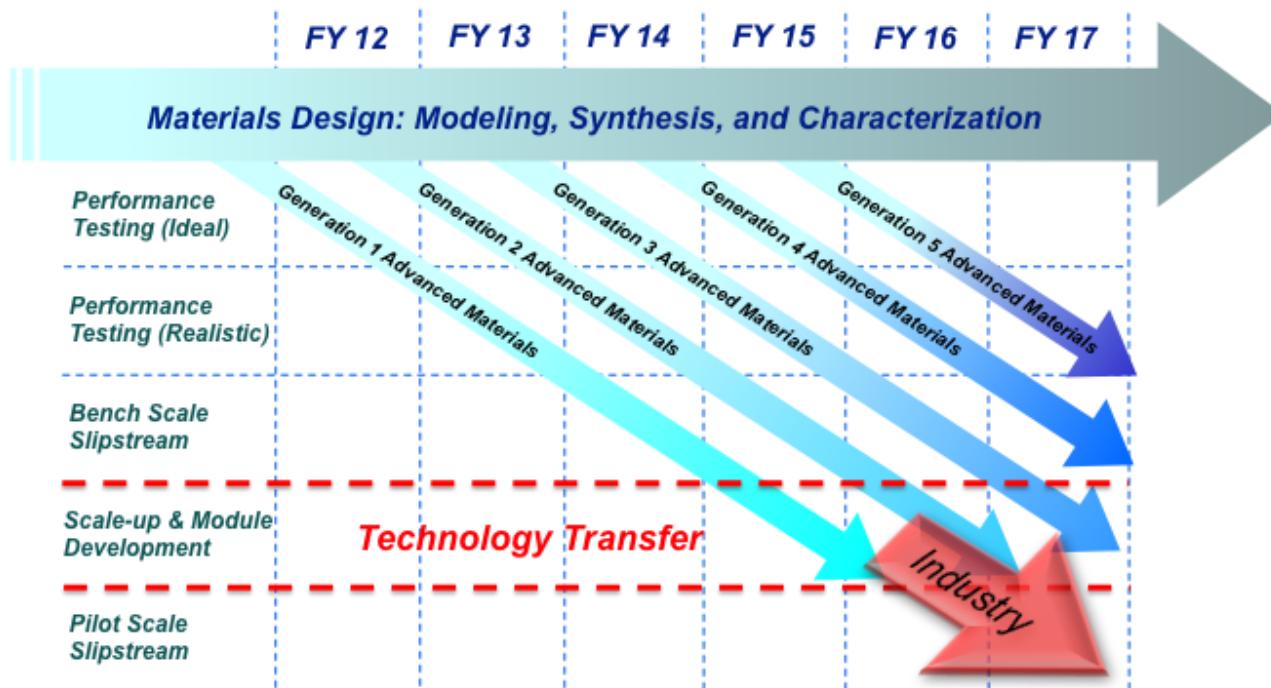
Key Challenges:

- Complex, integrated power process
- Additional process (WGS) to get high capture rates
- Current technology (Selexol) requires cooling and reheating

NETL-RUA Goals

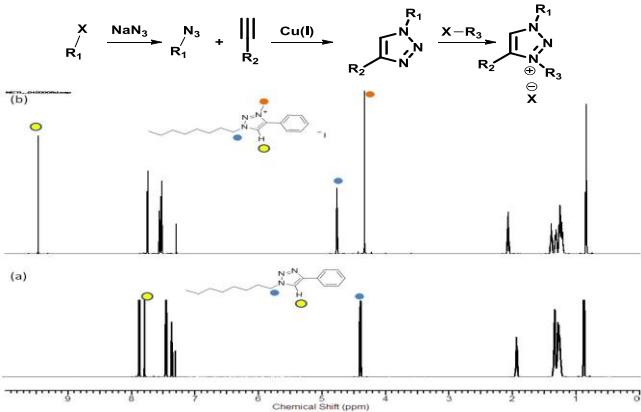
Research & Development Goal

- Accelerate the development of efficient, cost effective pre-, post-, and oxy-combustion carbon capture technology
 - Innovative technology development
 - Lab-scale assessment of emerging technology
 - Slip-stream testing of most promising technology

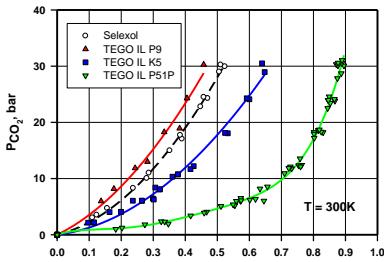


Integrated Materials Development

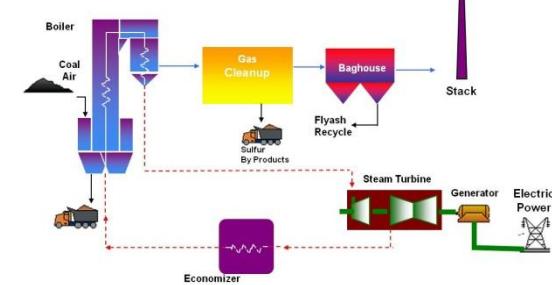
Characterization



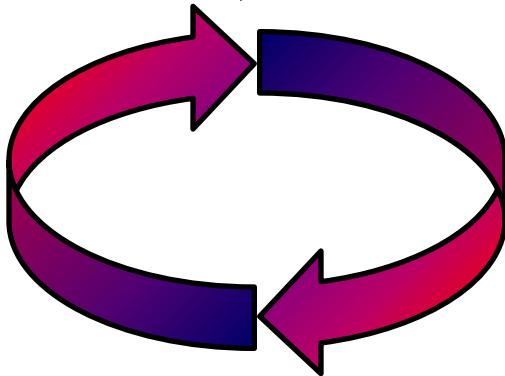
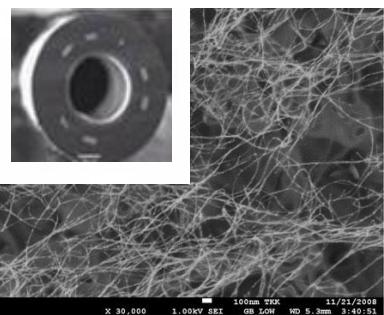
Performance Testing



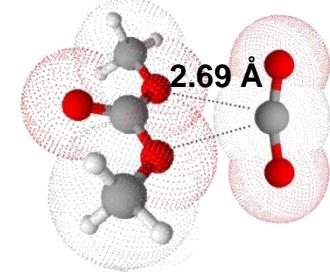
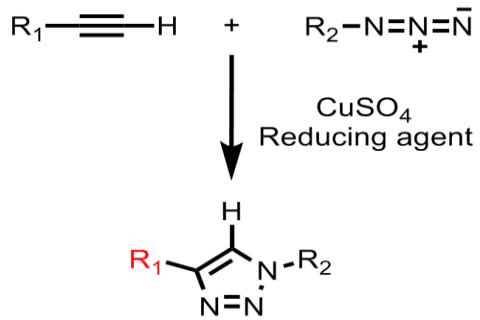
Systems Analysis



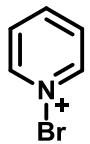
Fabrication



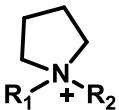
Synthesis



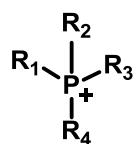
What is an ionic liquid?



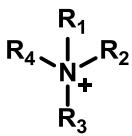
Pyridinium



Pyrrolidinium



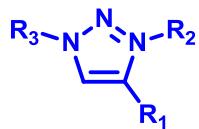
Phosphonium



Ammonium

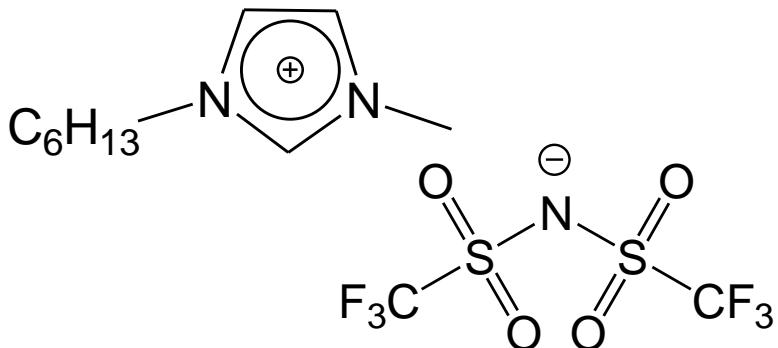


Imidazolium

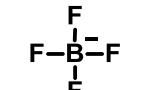


Triazolium

Estimated 10^{14} possible ionic liquids



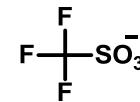
~1000 ionic liquids commercially available



Tetrafluoroborate



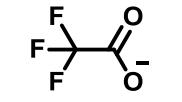
Hexafluorophosphate



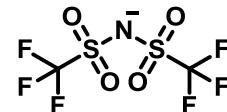
Trifluoromethylsulfonate



Acetate



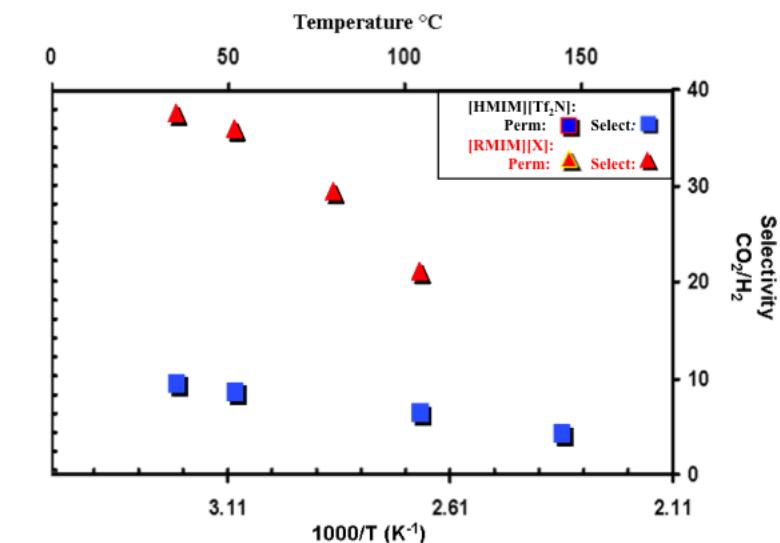
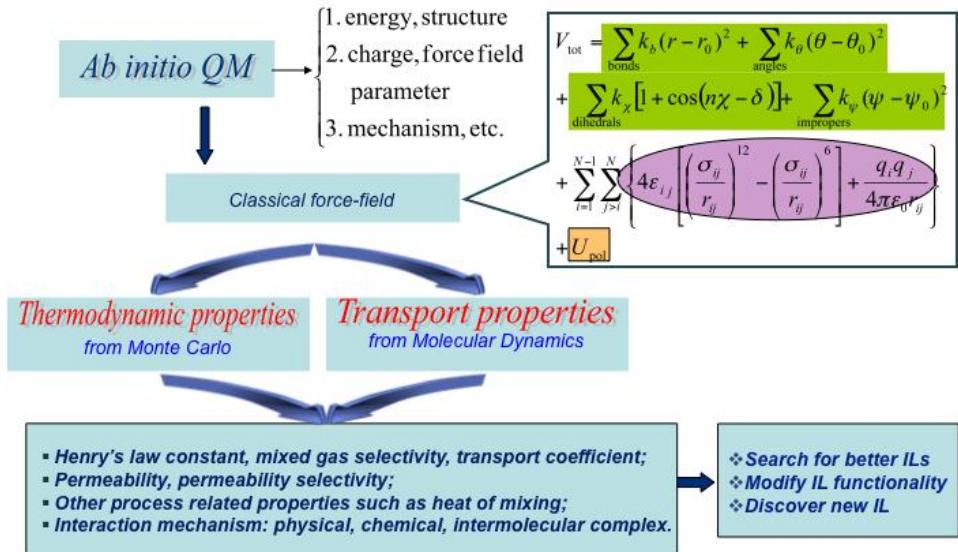
Trifluoroacetate

TF₂N

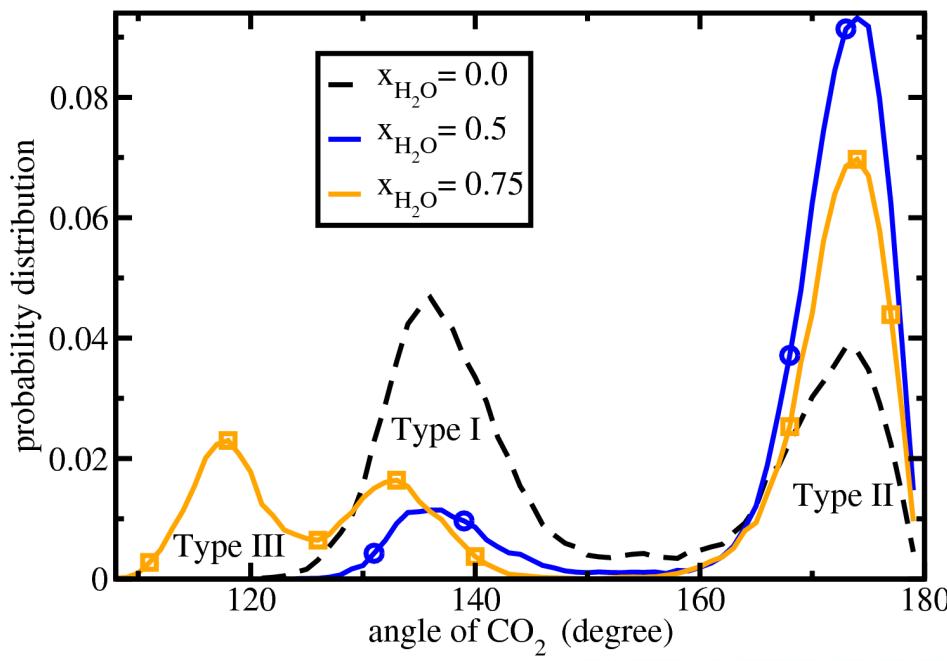
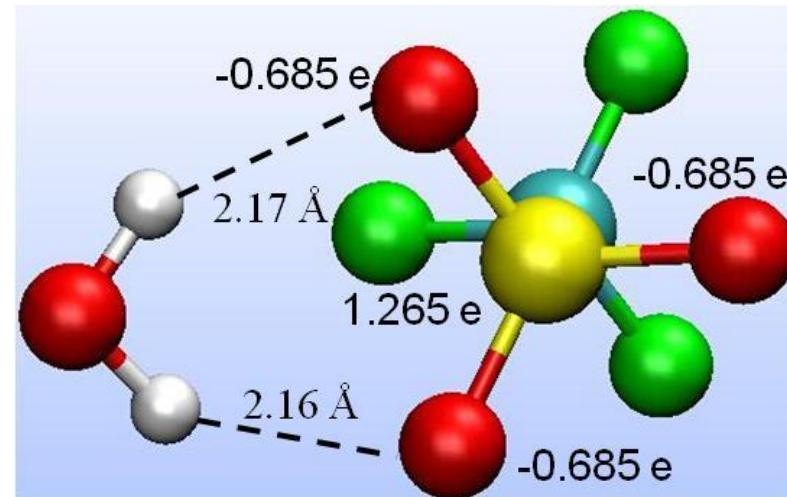
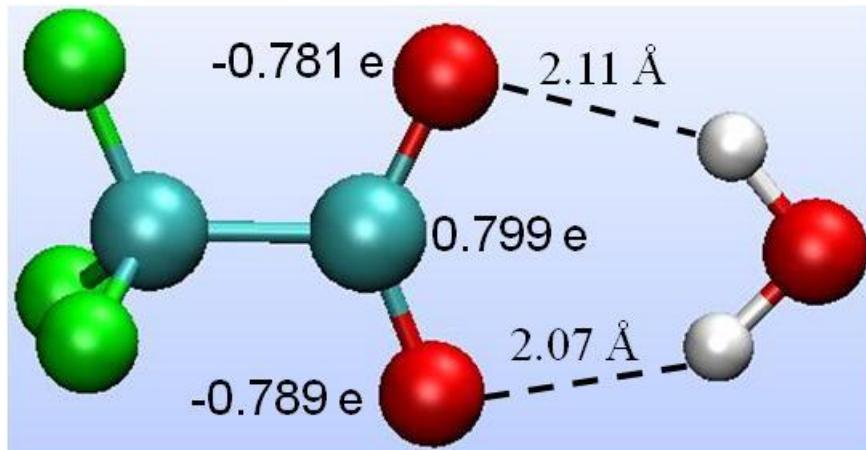
- Highly Tailorable Liquid Salts
 - Negligible Vapor Pressure
 - Good Thermal Stability
 - High CO₂ solubility relative to CH₄, N₂, and H₂

Modeling

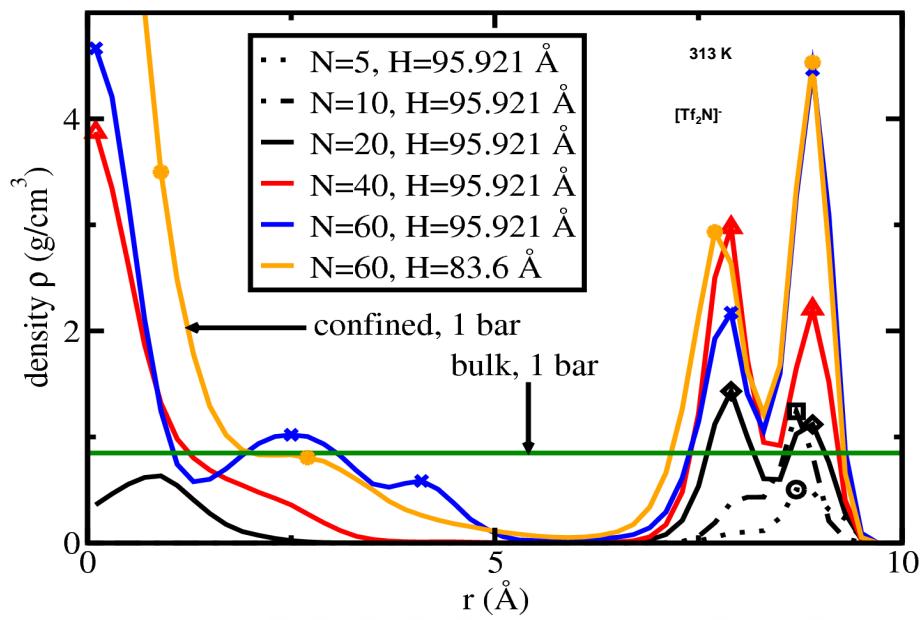
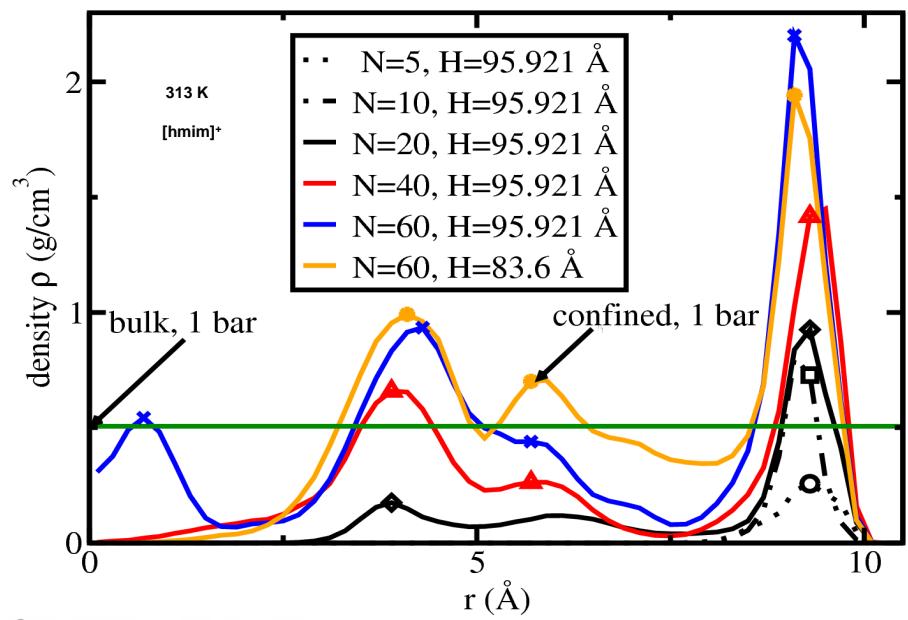
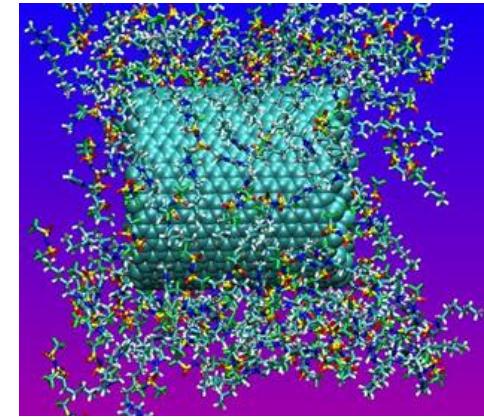
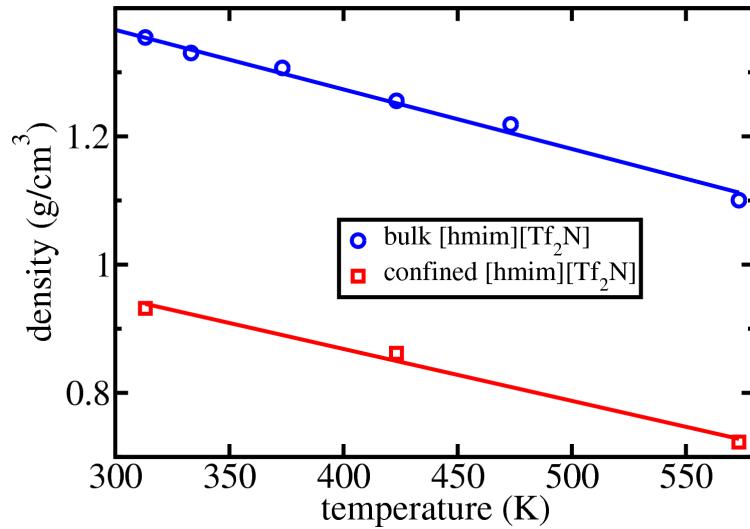
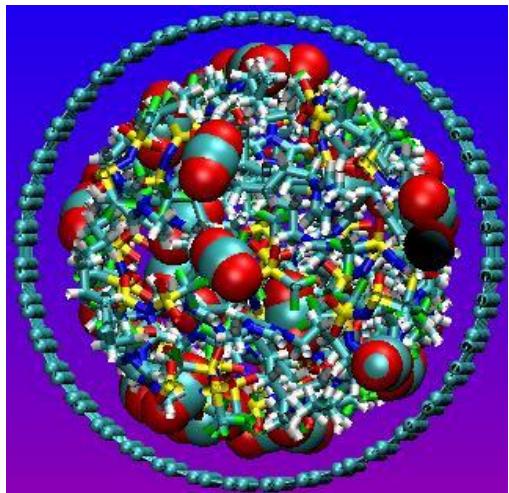
- **Force Field Development**
 - Inclusion of Polerizability
 - Development of Fields for Reactive ILs
- **Monte Carlo and molecular dynamics of IL/H₂O/CO₂ interactions**
- **Modeling of ILs contained in the pores of supports**
- **Implement chemical informatic approaches to search for promising IL structures**



Effect of Water

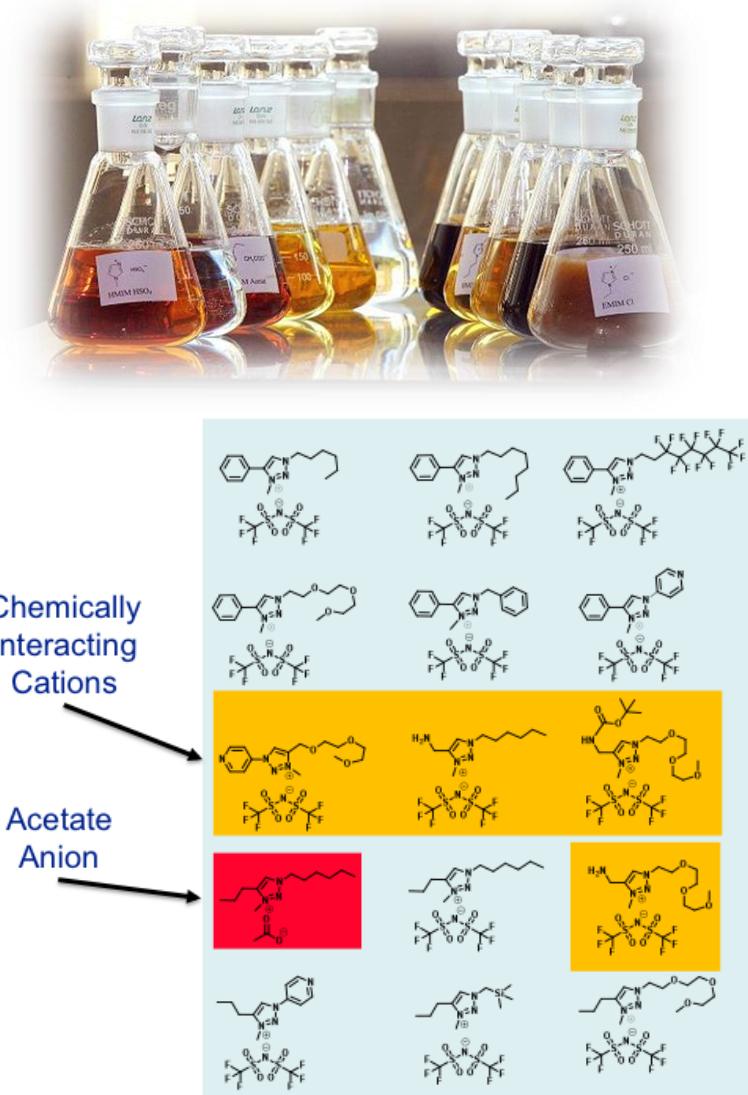


Confinement of ILs

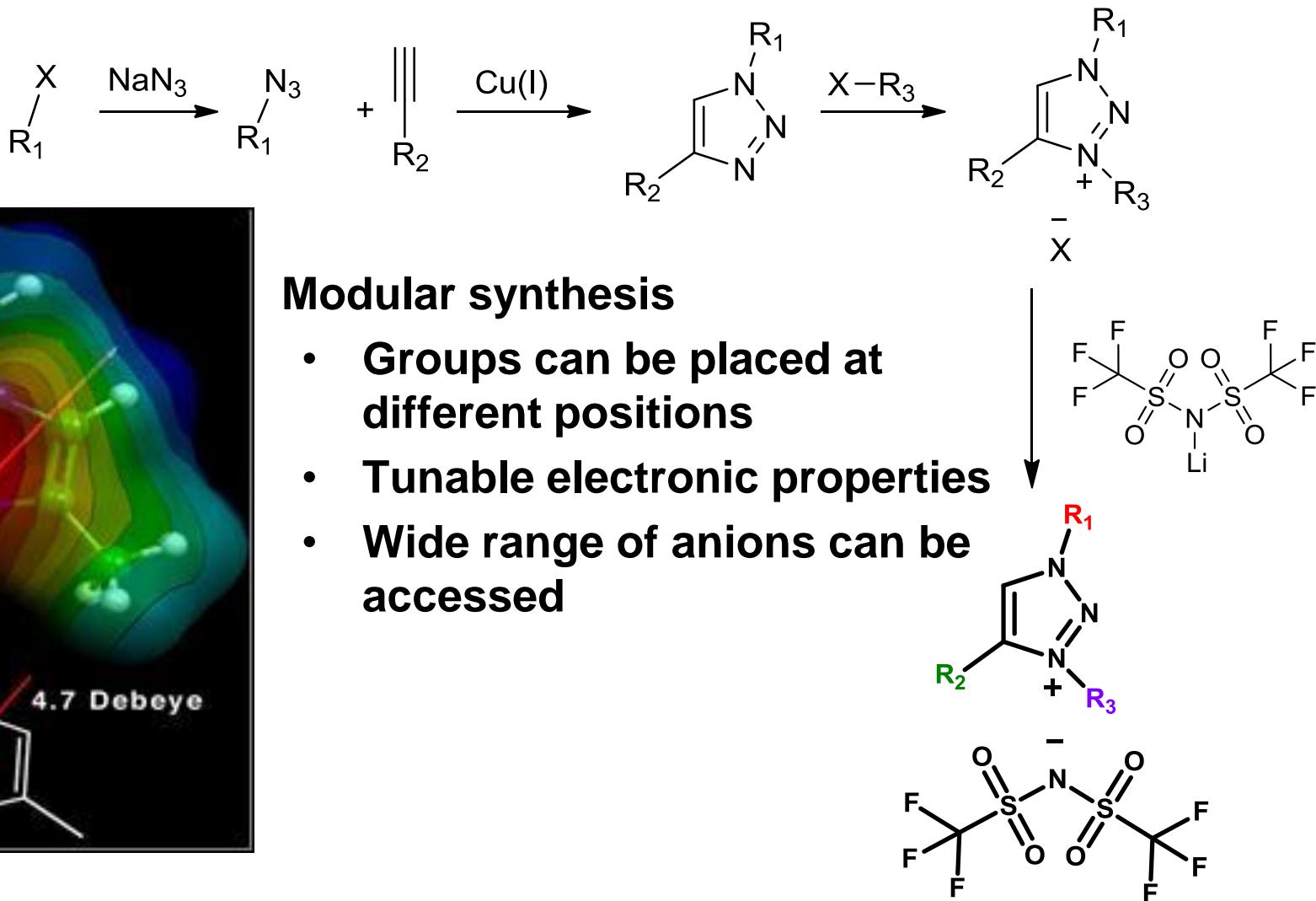


Synthesis

- **Synthesize Promising Candidate ILs Suggested by Modeling**
- **Prepare Triazolium ILs and Continue Elucidation of the Effect of the Cation**
 - Regioisomers
- **Develop Multivalent ILs and Structured Complex ILs**

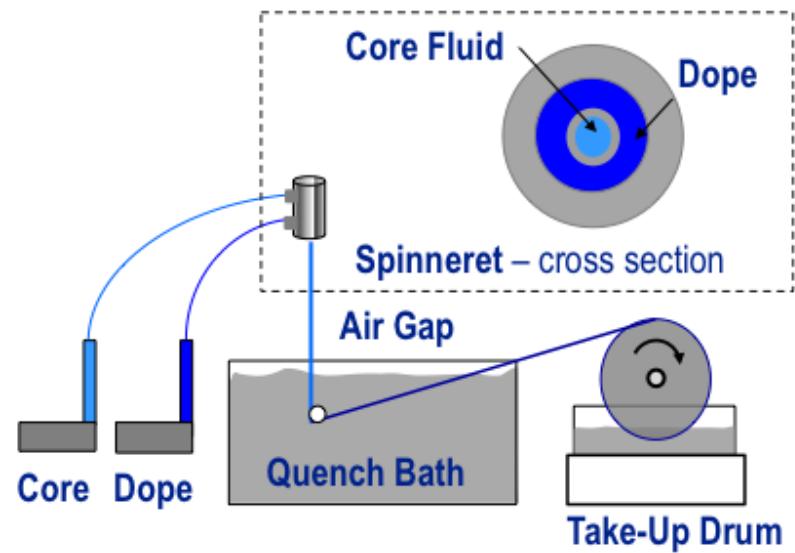
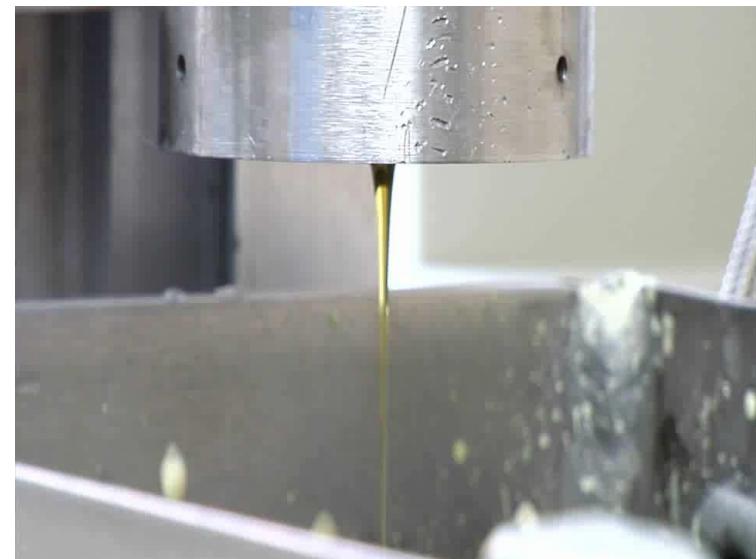
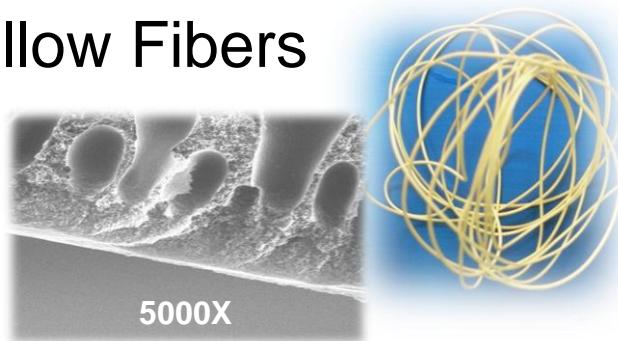


Synthesis of Triazolium IL

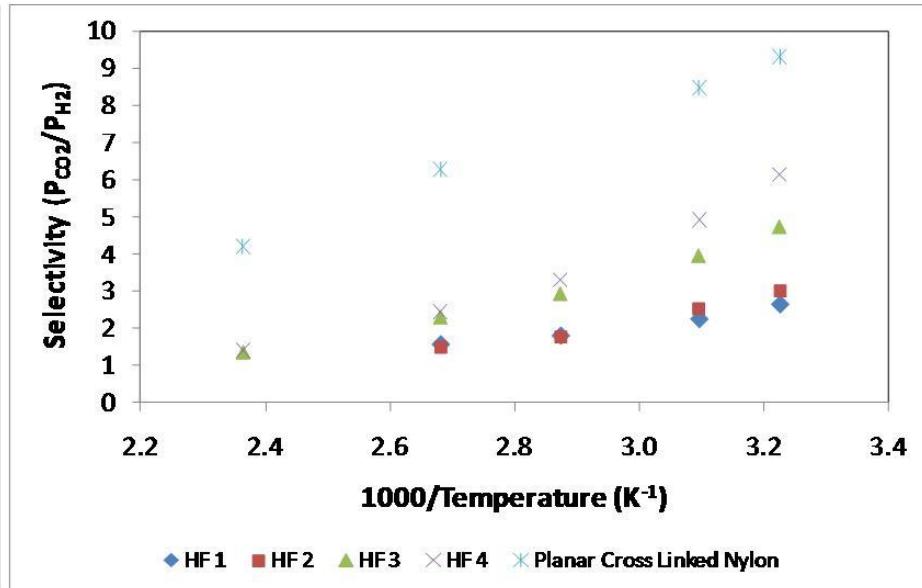
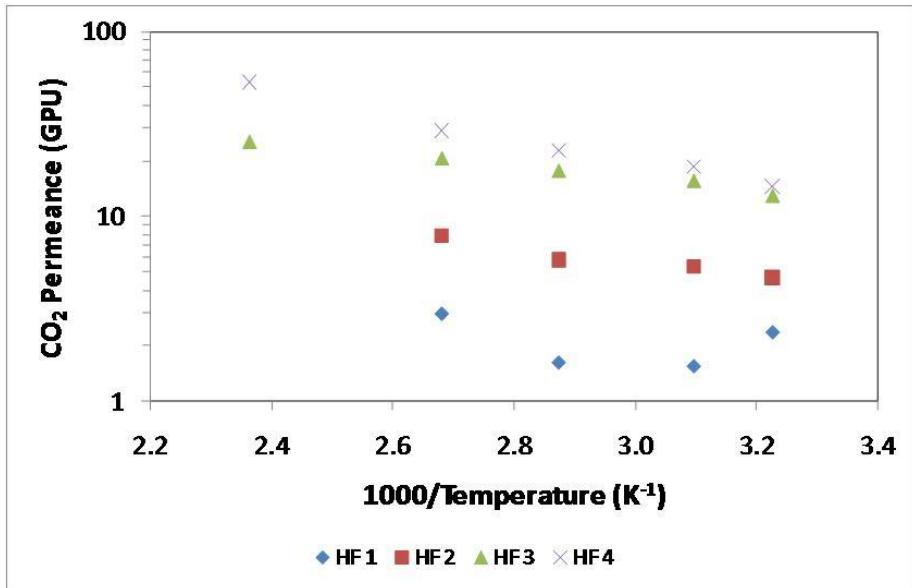
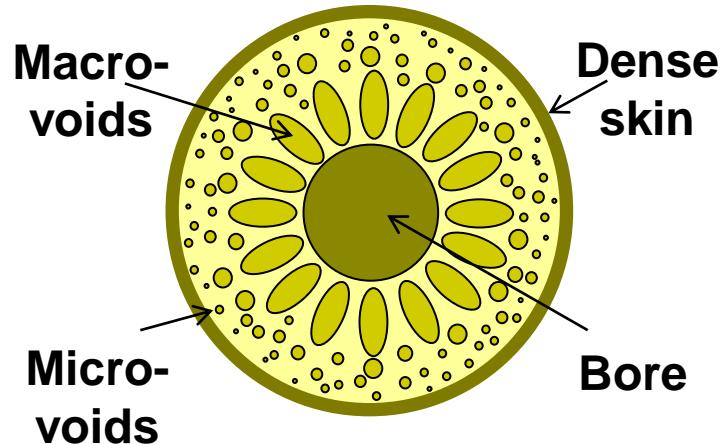
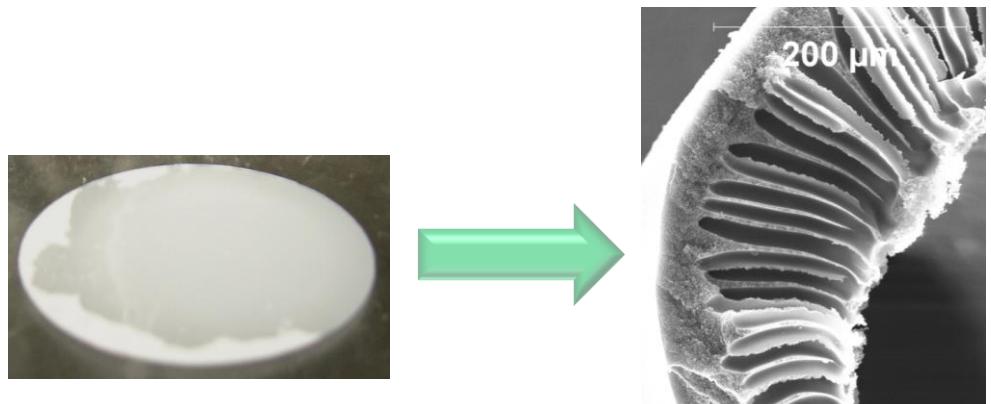


Fabrication

- Optimize IL-containing Hollow Fiber Fabrication
- Examine the Mechanical Stability of SILMs
 - Coupons
 - Hollow Fibers

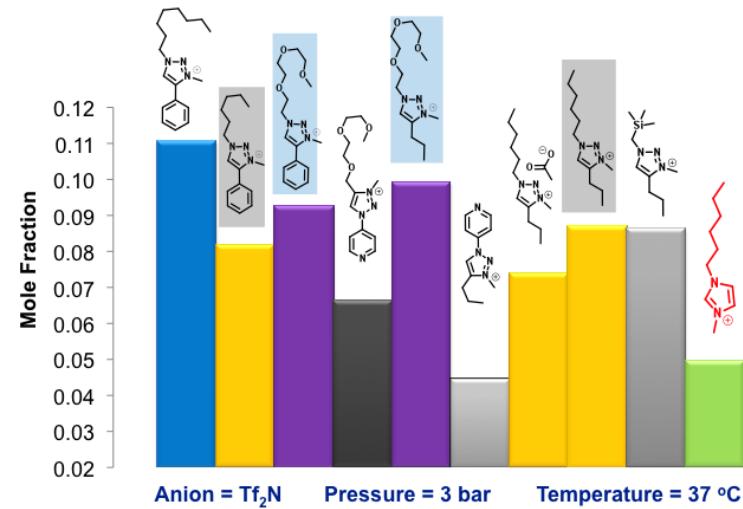
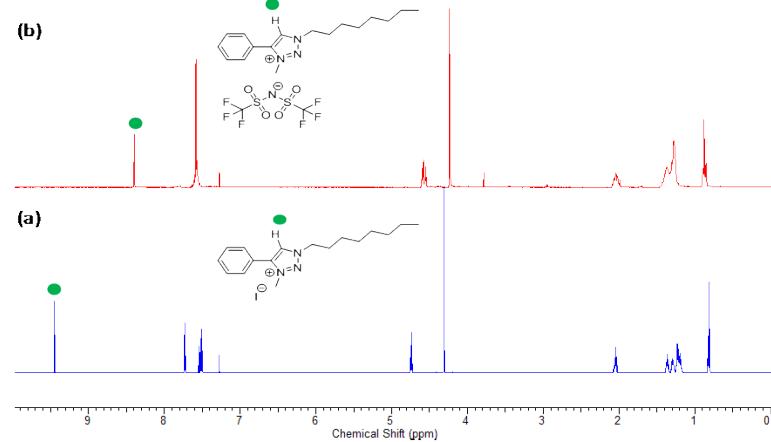


IL-containing Hollow Fibers

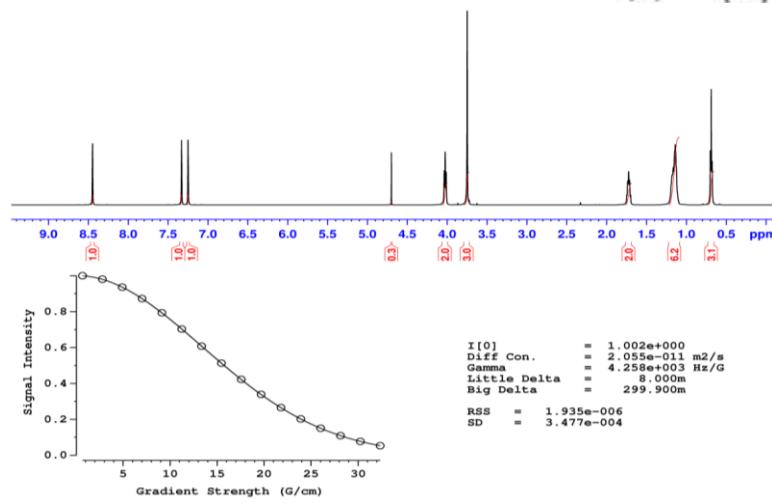
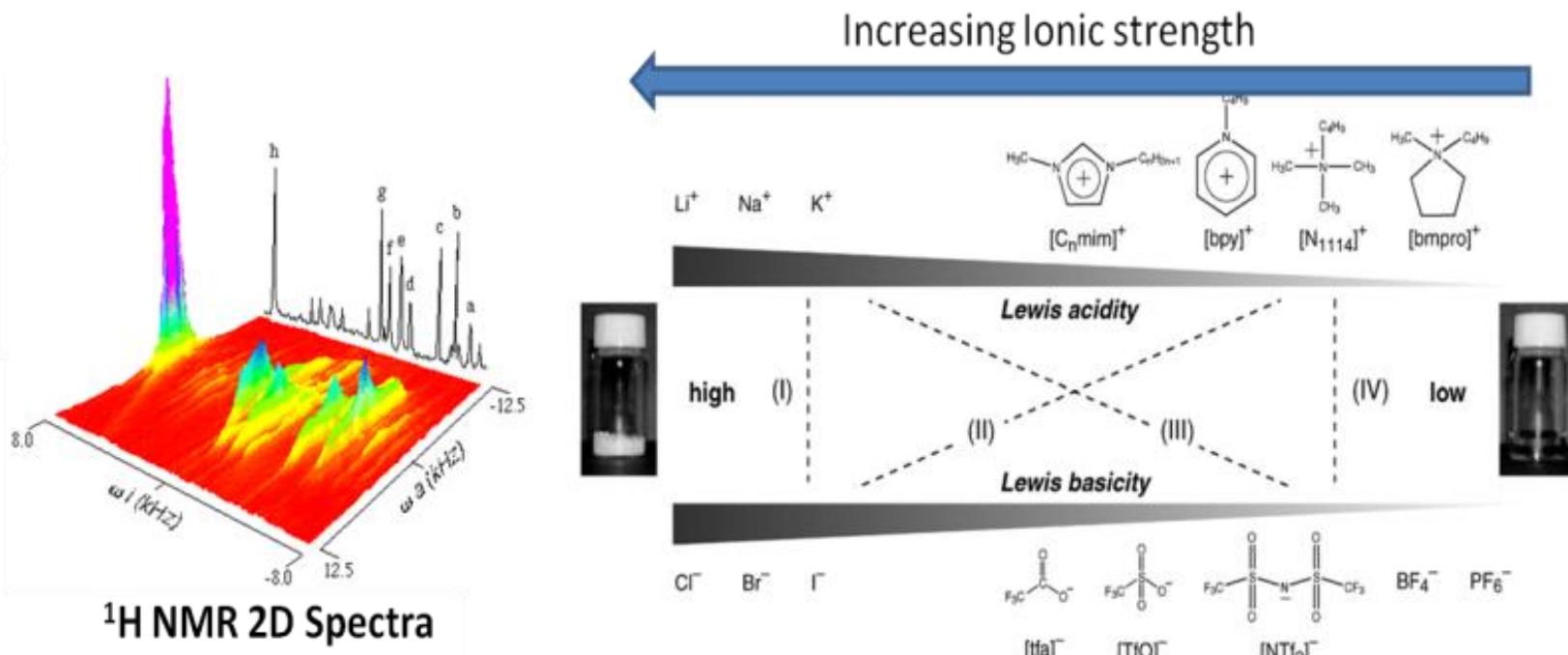


Characterization

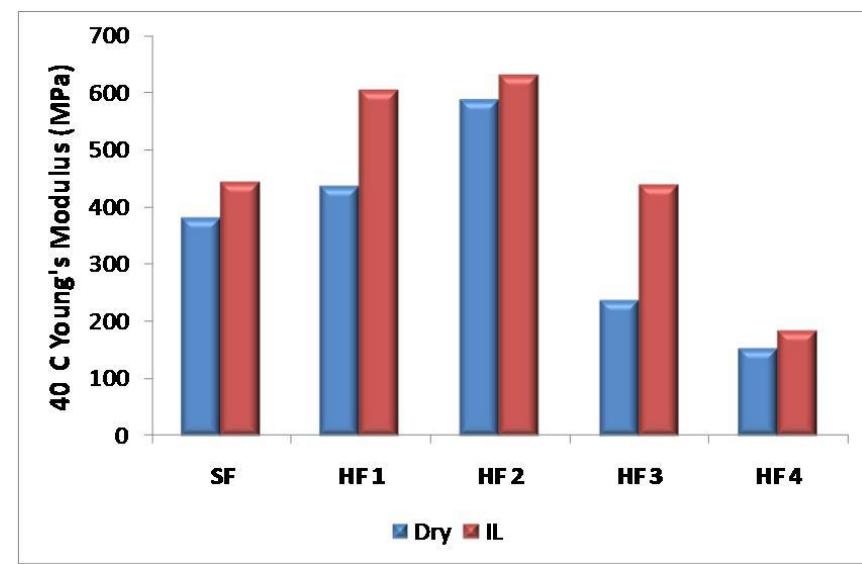
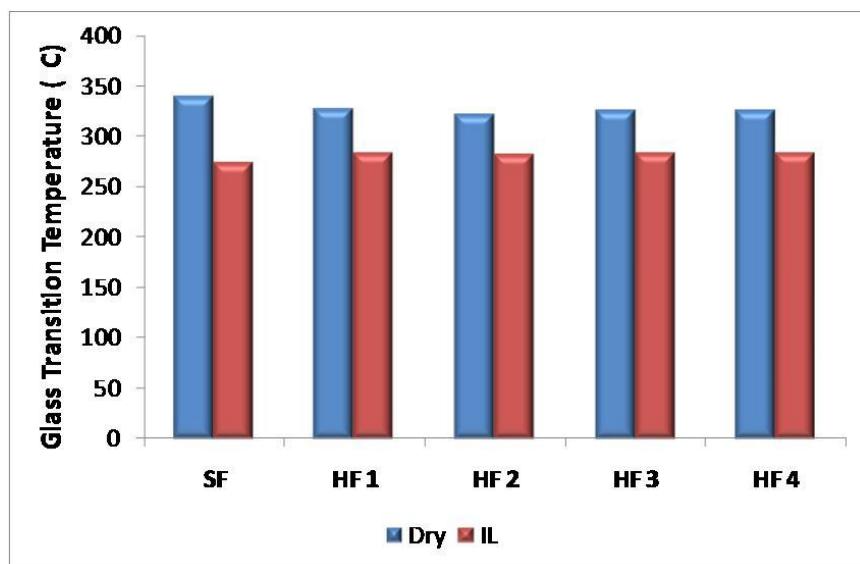
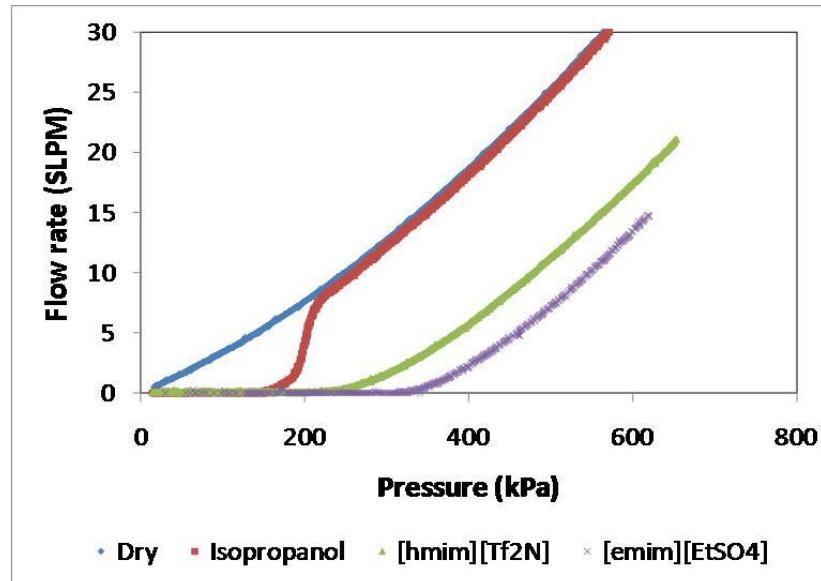
- **Probe ILs Using Soft X-ray Spectroscopic Techniques**
 - Interaction of CO₂ and Other Gases
 - Nano-scale Heterogeneity
- **Elucidate Inductive Effects on CO₂ Solubility**
 - NMR Peak Shift
 - Ionicity



Correlation of Physical Properties

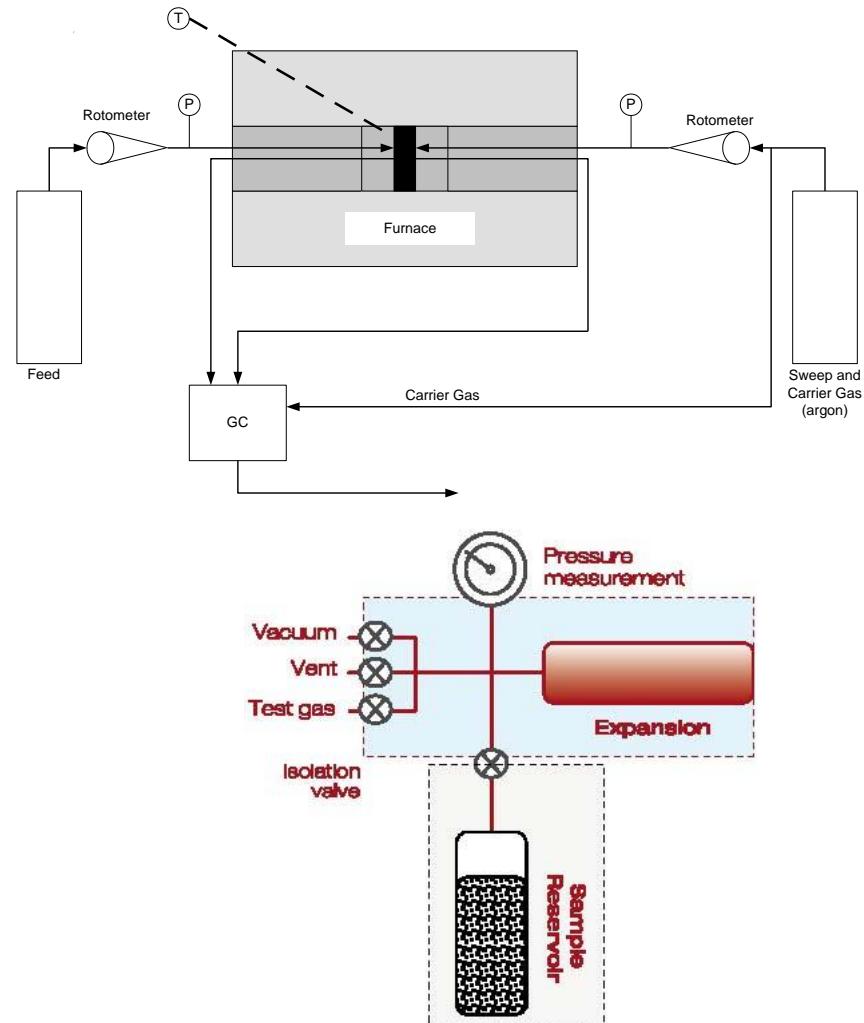


Fiber Mechanical Properties



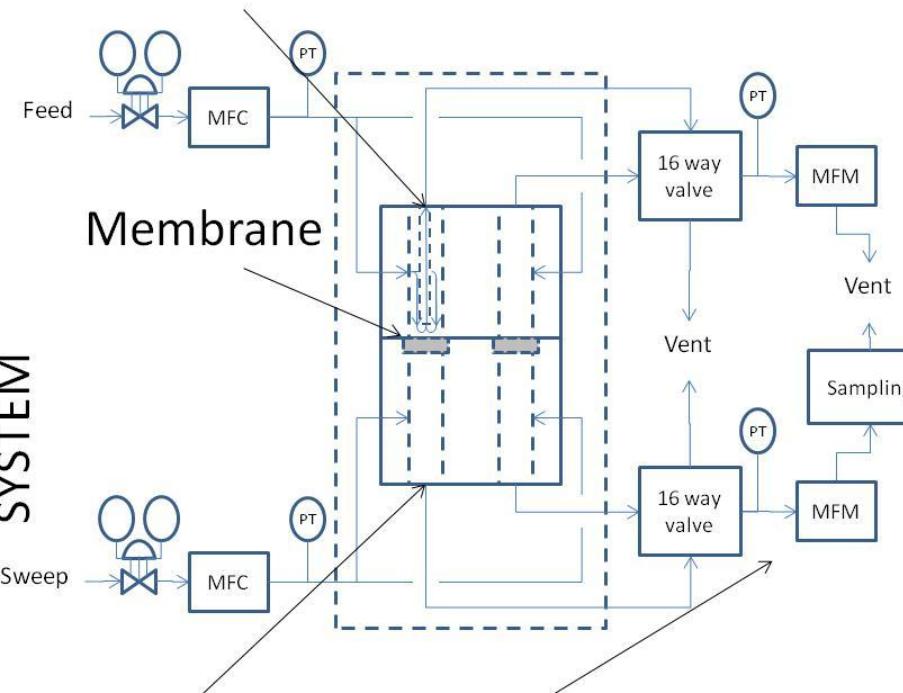
Performance Testing

- Examine the Solubility of CO₂ in Novel ILs to Screen for Applicability as Solvents
- Measure the Membrane Performance Properties of SILMs Based on Novel ILs
- Develop a High-throughput Membrane Screening System



High Throughput Membrane Screening

Feed Gas



SYSTEM

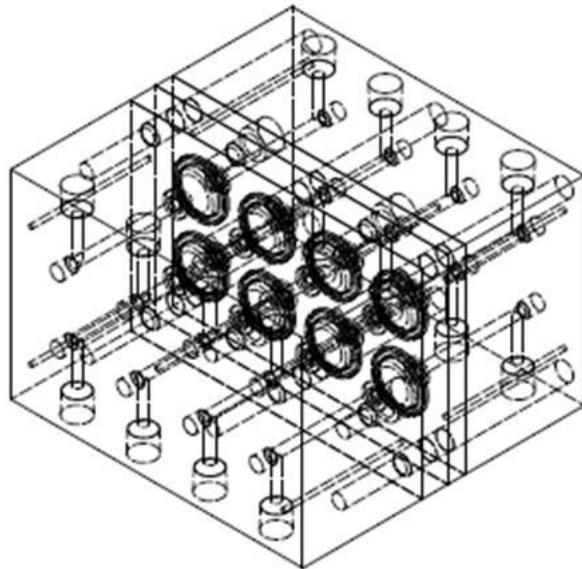
Permeate Gas

Pressure, Flow, and
Concentration
Measurement

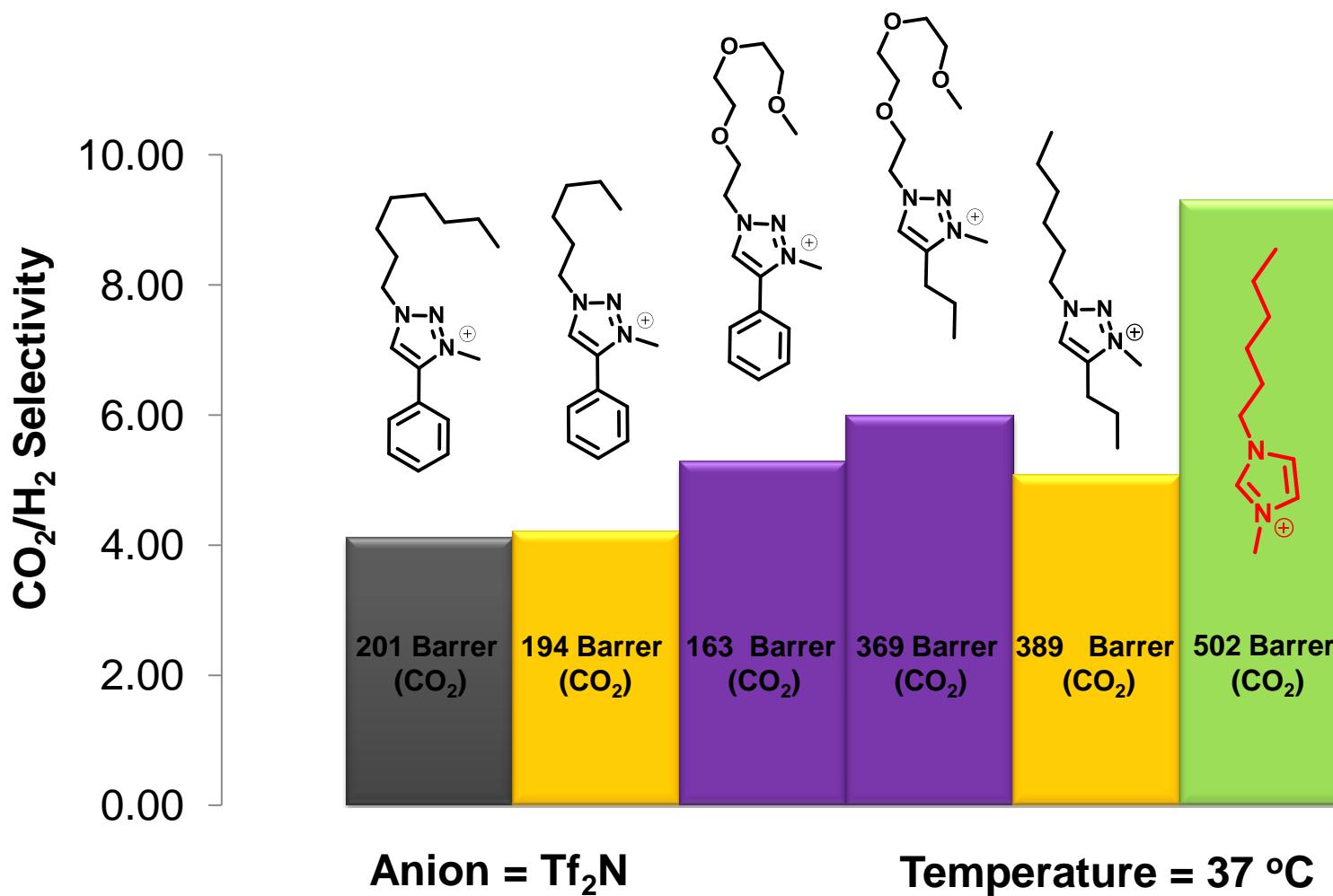
1 MOFs
5 Crystal Sizes
10 Loadings → 50 Membrane Tests Required

	Days/test	Membranes/test	Membranes tested/day	Days to test 50 membranes
Single Cell System	3	1	0.33	150
HT System	4	16	4	12.5

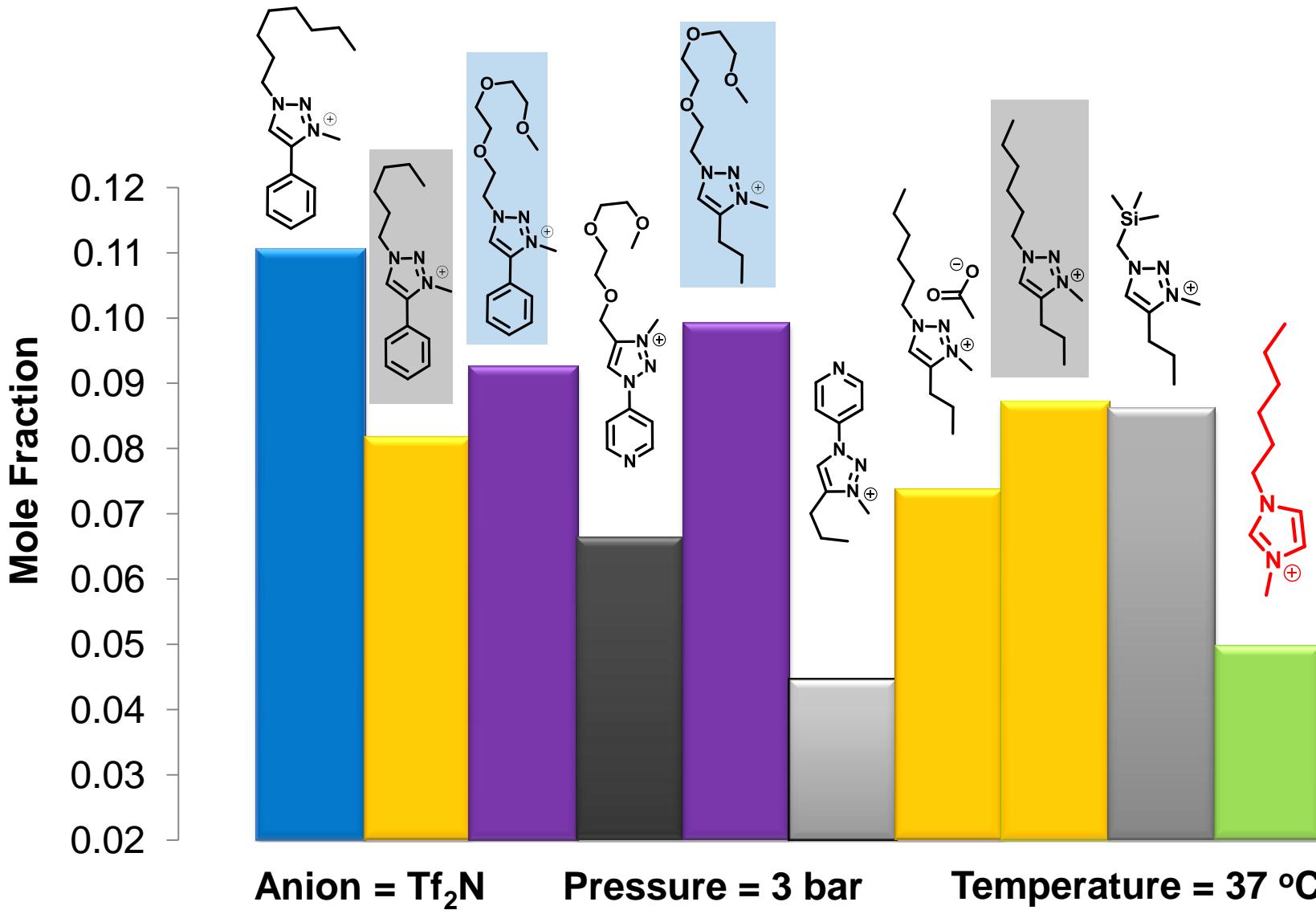
8-CELL BLOCK



Membrane Performance



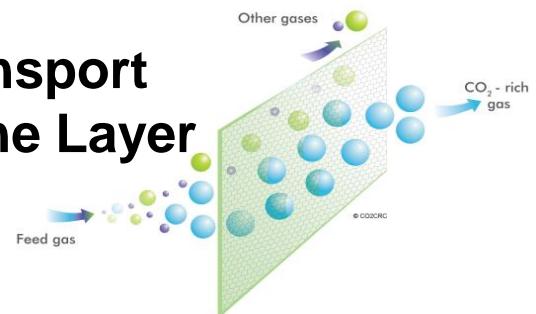
CO_2 Solubility (Molar Basis)



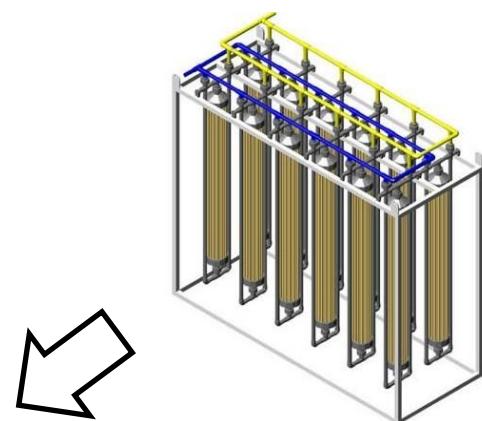
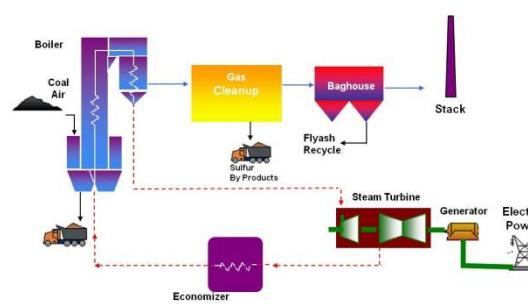
Systems Analysis

- Assemble a Team of Researchers and Systems Analysts to Examine CO₂-selective Membranes in Power Generation Applications
- Begin Multi-scale Systems Analysis
 - Membrane Layer
 - Module
 - Power Plant

Semi-empirical Transport Modeling of Membrane Layer

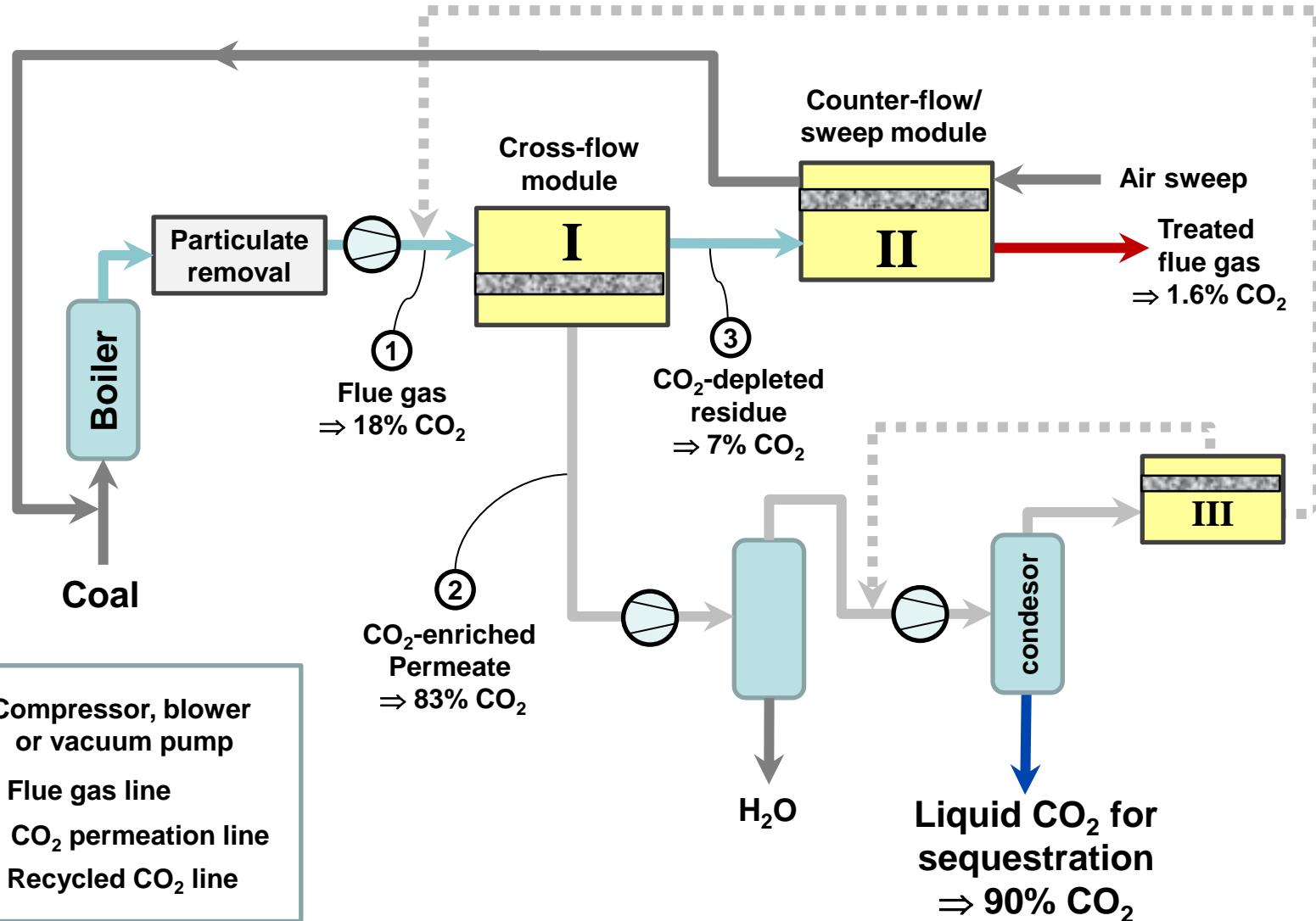


Computational Fluid Dynamics Modeling of Module



Process Simulation of Power Plant

Two-Step Counter-Flow/Sweep Design



NETL's Office of Research & Development Contacts

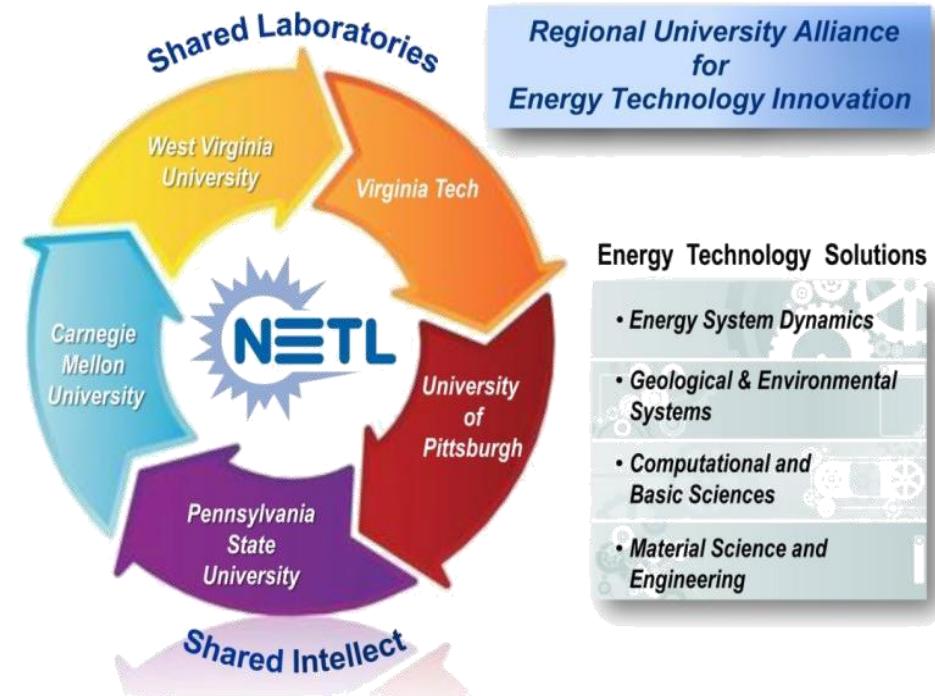
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FOSSIL ENERGY NEWS SPOTLIGHT

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A groundbreaking Department of Energy-developed imaging system originally designed to help create cleaner fossil energy processes is finding successful applications in a wide range of medical, chemical processing, energy, and other industries. [Read More >](#)

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the ENERGY lab
Where energy challenges converge and energy solutions emerge



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A groundbreaking DOE-developed imaging system originally designed to help create cleaner fossil energy processes is finding successful applications in a wide range of other industries. [Read More!](#)

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NEWS

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[Read More about NETL's 100 Years!](#)

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[Major CO₂ Geologic Storage Formations](#)
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